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Sodium dipotassium citrate, $NaK_2C_6H_5O_7$

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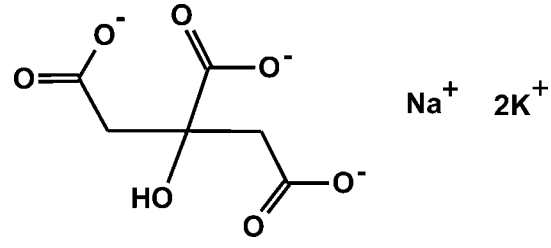
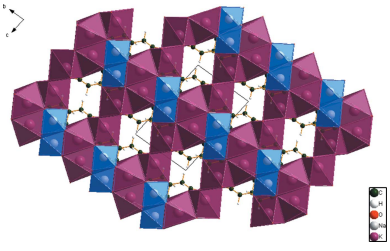
The crystal structure of sodium dipotassium citrate, $Na^+{\cdot}2K^+{\cdot}C_6H_5O_7^{3-}$, has been solved and refined using laboratory X-ray powder diffraction data, and optimized using density functional techniques. The Na^+ and one of the K^+ cations are six-coordinate, with bond-valence sums of 1.13 and 0.92 valence units, respectively, while another crystallographically independent K^+ cation is seven-coordinate with a bond-valence sum of 1.20. The $[KO_6]$ and $[KO_7]$ polyhedra share edges and corners to form layers perpendicular to the *b* axis. The distorted $[NaO_6]$ octahedra share edges to form chains along the *a* axis. The result is a three-dimensional network. The only O—H···O hydrogen bond is an intramolecular one between the hydroxy group and a terminal carboxylate group.

1. Chemical context

We have carried out a systematic study of the crystal structures of Group 1 (alkali metal) citrate salts to understand the anion's conformational flexibility, ionization, coordination tendencies, and hydrogen bonding. Most of the new structures were solved using powder diffraction data (laboratory and/or synchrotron), but single crystals were used where available. The general trends and conclusions about the 16 new compounds and 12 previously characterized structures are being reported separately (Rammohan & Kaduk, 2016*a*). The initial study considered salts containing one type of Group 1 cations. This compound (Fig. 1) represents an extension of the study to salts containing more than one alkali metal cation. The structure of related sodium potassium hydrogen citrate has been published recently (Rammohan & Kaduk, 2016*b*).





2. Structural commentary

The root-mean-square deviation of the non-hydrogen atoms in the refined and optimized structures is only 0.069 Å. The excellent agreement between the structures (Fig. 2) is strong evidence that the experimental structure is correct (van de Streek & Neumann, 2014). This discussion uses the DFT-optimized structure. All of the bond lengths and torsion angles, and most of the bond angles fall within the normal

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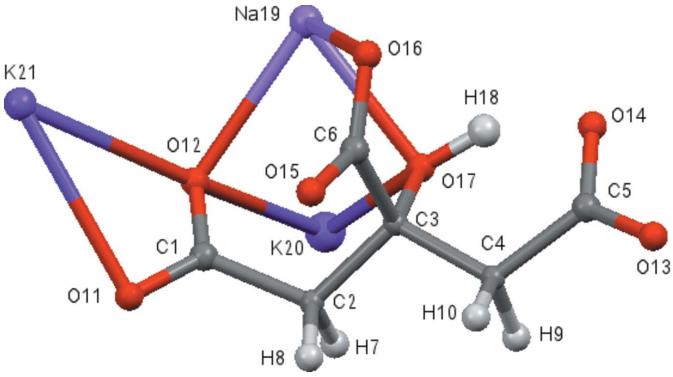

Figure 1
The content of asymmetric unit of the title compound showing the atom numbering and 50% probability displacement spheroids.

ranges indicated by a *Mercury Mogul* Geometry Check (Macrae *et al.*, 2008). Only the O17—C3—C4 [observed = 115.4 (4), optimized = 109.3, normal = 110.6 (3)°, Z-score = 4.9] and O17—C3—C6 [observed = 109.0 (3), optimized = 111.4, normal = 105.4 (6)°, Z-score = 10.5] angles are flagged as unusual. Part of the reason for the high Z-scores is the exceptionally low standard uncertainties on the normal values. The hydroxy group O17–H18 bridges Na19 and K20, so a small distortion from the normal geometry may be expected. The citrate anion occurs in the *trans,trans*-conformation (about C2—C3 and C3—C4), which is one of the two low-energy conformations of an isolated citrate. The central carboxylate group and the hydroxy group occur in the normal planar arrangement. The citrate chelates to Na19 through the terminal carboxylate oxygen O12, the central carboxylate oxygen O17, and the hydroxy oxygen O17. The citrate chelates to K20 through the terminal carboxylate oxygen O12 and the hydroxy oxygen O17. One terminal carboxylate group (C1/O11/O12) chelates to K21. Na19 is six-coordinate (distorted octahedral), with a bond-valence sum of 1.13 valence units (v.u.). K20 is also six-coordinate with a bond-valence sum of 0.92 v.u.; K21 is seven-coordinate, with a bond-valence sum of 1.20 v.u. Na19 and K21 are thus slightly crowded, while K20 is slightly underbonded. The metal–oxygen bonding is ionic, based on the cation charges and Mulliken overlap populations.

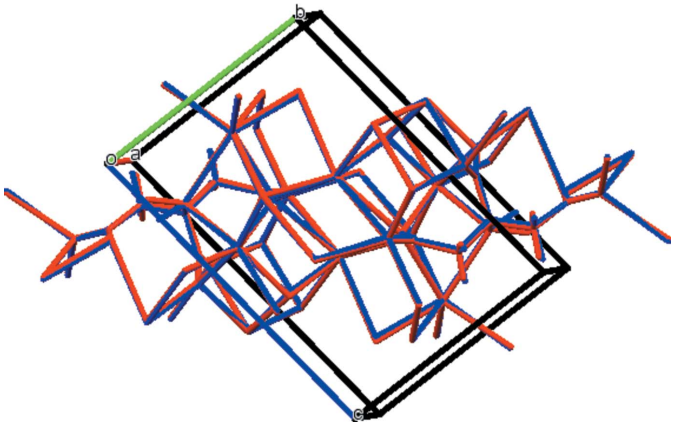

Figure 2
Comparison of the refined and optimized structures of sodium dipotassium citrate. The refined structure is in red, and the DFT-optimized structure is in blue.

Table 1
Hydrogen-bond geometry (Å, °) for the DFT-optimized structure.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O17—H18···O14	0.989	1.721	2.614	148.2
C2—H7···O13	1.095	2.480	3.448	165.8
C2—H8···O17	1.089	2.382	3.513	149.0

3. Supramolecular features

In the crystal structure (Fig. 3), the [KO_6] and [KO_7] polyhedra share edges and corners to form layers perpendicular to the *b* axis. The distorted [NaO_6] octahedra share edges to form chains along the *a* axis. The result is a three-dimensional network. The only O—H···O hydrogen bond is an intramolecular one, O17—H18···O14 (Table 1), between the hydroxy group and a terminal carboxylate. Two intermolecular C—H···O hydrogen bonds also apparently contribute to the crystal energy.

4. Database survey

Details of the comprehensive literature search for citrate structures are presented in Rammohan & Kaduk (2016*a*). A reduced cell search in the Cambridge Structural Database (Groom & Allen, 2014) (increasing the default tolerance from 1.5 to 2.0%, to account for the differences between ambient and low-temperature lattice parameters) yielded 25 hits, but limiting the chemistry to C, H, O, Na, and K only resulted in no hits. The powder pattern matched no entry in the Powder Diffraction File (ICDD, 2015).

5. Synthesis and crystallization

2.0764 g (10.0 mmol) $H_3C_6H_5O_7(H_2O)$ was dissolved in 20 ml deionized water. 0.5365 g Na_2CO_3 (10.0 mmol Na, Sigma–

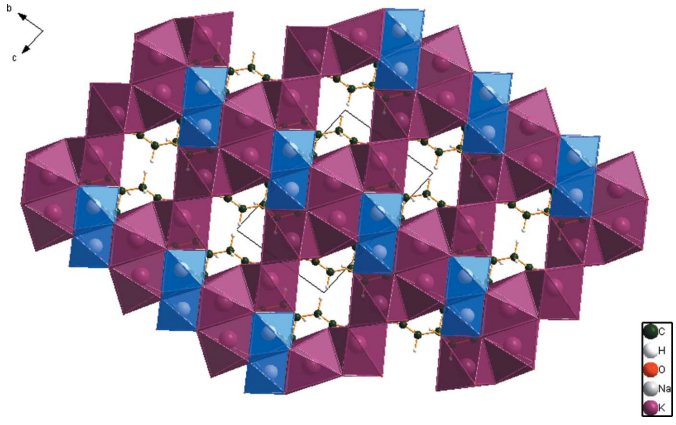

Figure 3
Crystal structure of $NaK_2C_6H_5O_7$, viewed approximately down the *a* axis.

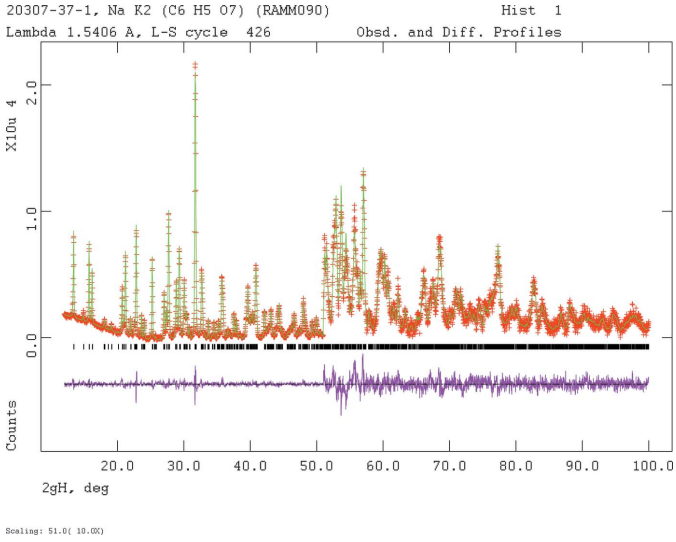

Figure 4
Rietveld plot for the refinement of $NaK_2C_6H_5O_7$. The red crosses represent the observed data points, and the green line is the calculated pattern. The magenta curve is the difference pattern, plotted at the same scale as the other patterns. The vertical scale has been multiplied by a factor of 10 for $2\theta > 51.0°$. The row of black tick marks indicates the Bragg reflection positions for the phase.

Aldrich) and 1.3824 g K_2CO_3 (20.0 mmol K, Sigma–Aldrich) were added to the citric acid solution slowly with stirring. The resulting clear colorless colution was evaporated to dryness in a 393 K oven.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. The powder pattern (Fig. 4) was indexed using *Jade 9.5* (MDI, 2012), which yielded a primitive triclinic unit cell with two formula units and with the lattice parameters as given in Table 2. Pseudovoigt profile coefficients were as parameterized in Thompson *et al.* (1987), and the asymmetry correction of Finger *et al.* (1994) was applied and microstrain broadening by Stephens (1999). The structure was solved with *FOX* (Favre-Nicolin & Černý, 2002) using a citrate, Na, and two K as fragments. One of the 10 solutions (2×10^6 moves, with a bump penalty with weighting factor = 50) yielded a much lower cost function than the others. All C—C and C—O bond lengths were restrained, as were all bond angles. The hydrogen atoms were included at fixed positions, which were re-calculated during the course of the refinement. The U_{iso} parameters of C2, C3, and C4 were constrained to be equal, and those of H7, H8, H9, and H10 were constrained to be 1.3 times that of these carbon atoms. The U_{iso} parameters of C1, C5, C6, and the oxygen atoms were constrained to be equal, and that of H18 was constrained to be 1.3 times this value.

The Bravais–Friedel–Donnay–Harker (Bravais, 1866; Friedel, 1907; Donnay & Harker, 1937) morphology suggests that we might expect platy morphology for sodium dipotassium citrate, with {001} as the principal faces. A 2nd-order spherical harmonic preferred orientation model was included in the refinement. The texture index was only 1.006, indicating that preferred orientation was not significant in this rotated flat-plate specimen. The powder pattern is included in the Powder Diffraction File as entry 00-065-1254.

Table 2
Experimental details.

	Powder data
Crystal data	
Chemical formula	$Na^+{\cdot}2K^+{\cdot}C_6H_5O_7^{3-}$
M_r	290.29
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	5.51284 (12), 7.62583 (13), 11.37121 (14)
α, β, γ (°)	83.4276 (17), 88.991 (2), 84.3488 (16)
V (Å^3)	472.59 (1)
Z	2
Radiation type	$K\alpha_1$, $K\alpha_2$, λ = 1.540629, 1.544451 Å
Specimen shape, size (mm)	Flat sheet, 24 × 24
Data collection	
Diffractometer	Bruker D2 Phaser
Specimen mounting	Standard holder
Data collection mode	Reflection
Scan method	Step
2θ values (°)	$2\theta_{min}$ = 4.908 $2\theta_{max}$ = 99.914 $2\theta_{step}$ = 0.020
Refinement	
R factors and goodness of fit	R_p = 0.030, R_{wp} = 0.039, R_{exp} = 0.023, $R(F^2)$ = 0.042, χ^2 = 3.062
No. of parameters	87
No. of restraints	29
H-atom treatment	Only H-atom displacement parameters refined

The same symmetry and lattice parameters were used for the DFT calculation. Computer programs: *DIFFRAC* (Bruker, 2009), *PowDLL* (Kourkoumelis, 2013), *FOX* (Favre-Nicolin & Černý, 2002), *GSAS* (Larson & Von Dreele, 2004), *EXPGUI* (Toby, 2001), *DIAMOND* (Crystal Impact, 2015) and *publCIF* (Westrip, 2010).

6.1. Density functional geometry optimization

A density functional geometry optimization (fixed experimental unit cell) was carried out using *CRYSTAL09* (Dovesi *et al.*, 2005). The basis sets for the H, C, and O atoms were those of Gatti *et al.* (1994), the basis sets for Na and K were those of Dovesi *et al.* (1991). The calculation used 8 k-points and the B3LYP functional, and took about 41 h on a 2.8 GHz PC. The U_{iso} parameters from the Rietveld refinement were assigned to the optimized fractional coordinates.

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supporting information

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Computing details

Data collection: *DIFFRAC* (Bruker, 2009) for RAMM090_publ. Data reduction: *PowDLL* (Kourkoumelis, 2013) for RAMM090_publ. Program(s) used to solve structure: *FOX* (Favre-Nicolin & Černý, 2002) for RAMM090_publ. Program(s) used to refine structure: *GSAS* (Larson & Von Dreele, 2004) and *EXPGUI* (Toby, 2001) for RAMM090_publ. Molecular graphics: *DIAMOND* (Crystal Impact, 2015) for RAMM090_publ. Software used to prepare material for publication: *publCIF* (Westrip, 2010) for RAMM090_publ.

(RAMM090_publ) Sodium dipotassium citrate

Crystal data

$Na^+·2K^+·C_6H_5O_7^{3-}$
M_r = 290.29
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.51284 (12) Å
b = 7.62583 (13) Å
c = 11.37121 (14) Å
α = 83.4276 (17)°
β = 88.991 (2)°
γ = 84.3488 (16)°
V = 472.59 (1) Å^3
Z = 2
D_x = 2.040 Mg m^{-3}
$K\alpha_1$, $K\alpha_2$ radiation, λ = 1.540629, 1.544451 Å
T = 300 K
white
flat sheet, 24 × 24 mm
Specimen preparation: Prepared at 393 K and 101 kPa

Data collection

Bruker D2 Phaser diffractometer
Radiation source: sealed X-ray tube, Bruker D2 Phaser
Specimen mounting: standard holder
Data collection mode: reflection
Scan method: step
$2\theta_{min}$ = 4.908°, $2\theta_{max}$ = 99.914°, $2\theta_{step}$ = 0.020°

Refinement

Least-squares matrix: full
R_p = 0.030
R_{wp} = 0.039
R_{exp} = 0.023
$R(F^2)$ = 0.04230
χ^2 = 3.062
4701 data points

Profile function: CW Profile function number 4 with 27 terms Pseudovoigt profile coefficients as parameterized in P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83. Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994). J. Appl. Cryst.,27,892-900. Microstrain broadening by P.W. Stephens, (1999). J. Appl. Cryst.,32,281-289. #1(GU) = 2.580 #2(GV) = 0.000 #3(GW) = 1.999 #4(GP) = 0.000 #5(LX) = 2.886 #6(ptec) = 0.00 #7(trns) = 4.34 #8(shft) = 1.7006 #9(sfec) = 0.00 #10(S/L) = 0.0168 #11(H/L) = 0.0200 #12(eta) = 0.9000 Peak tails are ignored where the intensity is below 0.0100 times the peak Aniso. broadening axis 0.0 0.0 1.0
87 parameters
29 restraints
Only H-atom displacement parameters refined
Weighting scheme based on measured s.u.'s
$(\Delta/\sigma)_{max}$ = 0.09
Background function: GSAS Background function number 1 with 6 terms. Shifted Chebyshev function of 1st kind 1: 1257.26 2: -666.506 3: 46.8166 4: 212.247 5: -159.806 6: 45.8742

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2359 (10)	0.6795 (12)	0.6968 (6)	0.0152 (11)*
C2	0.2042 (13)	0.7850 (8)	0.8016 (5)	0.011 (2)*
C3	0.3308 (9)	0.9576 (6)	0.7836 (4)	0.011 (2)*
C4	0.2348 (14)	1.0793 (9)	0.8767 (7)	0.011 (2)*
C5	0.3654 (11)	1.2454 (8)	0.8714 (9)	0.0152 (11)*
C6	0.2669 (10)	1.0520 (11)	0.6588 (5)	0.0152 (11)*
H7	0.28281	0.69951	0.88349	0.015 (3)*
H8	0.00182	0.82253	0.81715	0.015 (3)*
H9	0.25920	1.00290	0.96853	0.015 (3)*
H10	0.03259	1.12135	0.86133	0.015 (3)*
O11	0.0522 (11)	0.6188 (9)	0.6561 (6)	0.0152 (11)*
O12	0.4449 (11)	0.6462 (9)	0.6513 (6)	0.0152 (11)*
O13	0.2630 (12)	1.3811 (8)	0.9141 (7)	0.0152 (11)*
O14	0.5910 (10)	1.2399 (8)	0.8447 (6)	0.0152 (11)*
O15	0.0475 (11)	1.0713 (9)	0.6249 (6)	0.0152 (11)*
O16	0.4326 (12)	1.1231 (9)	0.5975 (5)	0.0152 (11)*
O17	0.5886 (10)	0.9166 (8)	0.7914 (5)	0.0152 (11)*
H18	0.63600	0.99510	0.84920	0.0198 (14)*
Na19	0.7450 (10)	0.8688 (6)	0.5942 (4)	0.0202 (19)*
K20	0.7634 (6)	0.5460 (4)	0.8652 (2)	0.0297 (13)*

K21	0.2569 (6)	0.6328 (4)	0.4134 (2)	0.0197 (14)*

Geometric parameters (Å, º)

C1—C2	1.5113 (17)	O14—K21^{vii}	3.111 (7)
C1—O11	1.269 (3)	O15—C6	1.265 (3)
C1—O12	1.270 (3)	O15—Na19^{i}	2.438 (8)
C2—C1	1.5113 (17)	O15—Na19^{vii}	2.732 (8)
C2—C3	1.5409 (17)	O15—K21^{viii}	2.674 (6)
C3—C2	1.5409 (17)	O16—C6	1.266 (3)
C3—C4	1.5405 (17)	O16—Na19	2.467 (7)
C3—C6	1.5461 (17)	O16—Na19^{vii}	2.397 (9)
C3—O17	1.420 (3)	O16—K21^{vii}	2.642 (7)
C4—C3	1.5405 (17)	O17—C3	1.427 (3)
C4—C5	1.5119 (17)	O17—Na19	2.442 (7)
C5—C4	1.5119 (17)	O17—K20	2.927 (6)
C5—O13	1.271 (3)	Na19—O11^{ix}	2.470 (7)
C5—O14	1.273 (3)	Na19—O12	2.510 (8)
C6—C3	1.5461 (17)	Na19—O15^{ix}	2.438 (8)
C6—O15	1.265 (3)	Na19—O15^{vii}	2.732 (8)
C6—O16	1.266 (3)	Na19—O16	2.467 (7)
O11—C1	1.270 (3)	Na19—O16^{vii}	2.397 (9)
O11—Na19^{i}	2.470 (7)	Na19—O17	2.442 (7)
O11—K20^{i}	2.869 (7)	K20—O11^{ix}	2.869 (7)
O11—K21	2.958 (7)	K20—O12	3.008 (7)
O11—K21^{ii}	2.872 (6)	K20—O13^{x}	3.158 (7)
O12—C1	1.270 (3)	K20—O13^{xi}	2.947 (7)
O12—Na19	2.510 (8)	K20—O13^{vi}	2.631 (7)
O12—K20	3.008 (7)	K20—O14^{x}	2.641 (6)
O12—K21	2.930 (7)	K20—O17	2.927 (6)
O12—K21^{iii}	2.720 (6)	K21—O11	2.958 (7)
O13—C5	1.271 (3)	K21—O11^{ii}	2.872 (6)
O13—K20^{iv}	2.947 (7)	K21—O12	2.930 (7)
O13—K20^{v}	3.158 (7)	K21—O12^{iii}	2.720 (6)
O13—K20^{vi}	2.631 (7)	K21—O14^{vii}	3.111 (7)
O14—C5	1.273 (3)	K21—O15^{viii}	2.674 (6)
O14—K20^{v}	2.641 (6)	K21—O16^{vii}	2.642 (7)
C2—C1—O11	119.5 (4)	O11^{ix}—Na19—O12	84.1 (2)
C2—C1—O12	120.8 (4)	O11^{ix}—Na19—O15^{ix}	88.6 (3)
O11—C1—O12	119.6 (4)	O11^{ix}—Na19—O15^{vii}	92.6 (2)
C1—C2—C3	112.7 (4)	O11^{ix}—Na19—O16	162.6 (3)
C2—C3—C4	109.3 (3)	O11^{ix}—Na19—O16^{vii}	117.3 (3)
C2—C3—C6	108.4 (4)	O11^{ix}—Na19—O17	97.2 (2)
C2—C3—O17	109.7 (4)	O12—Na19—O15^{ix}	156.9 (3)
C4—C3—C6	109.0 (4)	O12—Na19—O15^{vii}	125.1 (3)
C4—C3—O17	111.5 (4)	O12—Na19—O16	93.0 (3)
C6—C3—O17	109.0 (3)	O12—Na19—O16^{vii}	83.0 (3)

C3—C4—C5	112.5 (3)	O12—Na19—O17	72.3 (2)
C4—C5—O13	119.5 (4)	O15^{ix}—Na19—O15^{vii}	77.0 (3)
C4—C5—O14	120.1 (4)	O15^{ix}—Na19—O16	87.4 (2)
O13—C5—O14	119.2 (4)	O15^{ix}—Na19—O16^{vii}	119.6 (3)
C3—C6—O15	119.5 (4)	O15^{ix}—Na19—O17	87.0 (3)
C3—C6—O16	118.7 (4)	O15^{vii}—Na19—O16	103.0 (2)
O15—C6—O16	121.4 (4)	O15^{vii}—Na19—O16^{vii}	50.46 (15)
C1—O11—Na19^{i}	108.7 (6)	O15^{vii}—Na19—O17	161.0 (3)
C1—O11—K20^{i}	102.2 (5)	O16—Na19—O16^{vii}	79.2 (3)
C1—O11—K21	93.1 (4)	O16—Na19—O17	65.7 (2)
C1—O11—K21^{ii}	159.7 (7)	O16^{vii}—Na19—O17	135.0 (3)
Na19^{i}—O11—K20^{i}	87.8 (2)	O11^{ix}—K20—O12	69.11 (15)
Na19^{i}—O11—K21	90.9 (2)	O11^{ix}—K20—O13^{x}	133.6 (2)
Na19^{i}—O11—K21^{ii}	91.5 (2)	O11^{ix}—K20—O13^{xi}	72.12 (19)
K20^{i}—O11—K21	164.2 (2)	O11^{ix}—K20—O13^{vi}	139.3 (2)
K20^{i}—O11—K21^{ii}	77.6 (2)	O11^{ix}—K20—O14^{x}	105.4 (2)
K21—O11—K21^{ii}	86.72 (18)	O11^{ix}—K20—O17	78.9 (2)
C1—O12—Na19	125.6 (7)	O12—K20—O13^{x}	71.3 (2)
C1—O12—K20	102.6 (5)	O12—K20—O13^{xi}	136.8 (2)
C1—O12—K21	94.4 (4)	O12—K20—O13^{vi}	134.4 (2)
C1—O12—K21^{iii}	140.1 (7)	O12—K20—O14^{x}	79.4 (2)
Na19—O12—K20	84.1 (2)	O12—K20—O17	58.96 (18)
Na19—O12—K21	97.1 (3)	O13^{x}—K20—O13^{xi}	129.1 (2)
Na19—O12—K21^{iii}	94.3 (2)	O13^{x}—K20—O13^{vi}	86.4 (2)
K20—O12—K21	158.2 (3)	O13^{x}—K20—O14^{x}	43.33 (13)
K20—O12—K21^{iii}	77.6 (2)	O13^{x}—K20—O17	100.46 (18)
K21—O12—K21^{iii}	80.6 (2)	O13^{xi}—K20—O13^{vi}	88.1 (2)
C5—O13—K20^{iv}	126.4 (6)	O13^{xi}—K20—O14^{x}	93.4 (2)
C5—O13—K20^{v}	86.0 (3)	O13^{xi}—K20—O17	129.94 (18)
C5—O13—K20^{vi}	129.6 (8)	O13^{vi}—K20—O14^{x}	111.0 (2)
K20^{iv}—O13—K20^{v}	129.1 (2)	O13^{vi}—K20—O17	88.3 (2)
K20^{iv}—O13—K20^{vi}	91.9 (2)	O14^{x}—K20—O17	133.9 (2)
K20^{v}—O13—K20^{vi}	93.6 (2)	O11—K21—O11^{ii}	93.28 (18)
C5—O14—K20^{v}	111.1 (3)	O11—K21—O12	43.76 (12)
C5—O14—K21^{vii}	119.0 (7)	O11—K21—O12^{iii}	119.8 (2)
K20^{v}—O14—K21^{vii}	76.9 (2)	O11—K21—O14^{vii}	163.54 (19)
C6—O15—Na19^{i}	134.6 (7)	O11—K21—O15^{viii}	83.75 (19)
C6—O15—Na19^{vii}	83.2 (4)	O11—K21—O16^{vii}	105.00 (18)
C6—O15—K21^{viii}	129.5 (7)	O11^{ii}—K21—O12	126.6 (2)
Na19^{i}—O15—Na19^{vii}	103.0 (3)	O11^{ii}—K21—O12^{iii}	73.16 (16)
Na19^{i}—O15—K21^{viii}	95.6 (2)	O11^{ii}—K21—O14^{vii}	94.23 (18)
Na19^{vii}—O15—K21^{viii}	91.77 (18)	O11^{ii}—K21—O15^{viii}	99.4 (2)
C6—O16—Na19	101.0 (5)	O11^{ii}—K21—O16^{vii}	161.3 (2)
C6—O16—Na19^{vii}	98.5 (5)	O12—K21—O12^{iii}	99.42 (19)
C6—O16—K21^{vii}	145.0 (7)	O12—K21—O14^{vii}	136.5 (2)
Na19—O16—Na19^{vii}	100.8 (3)	O12—K21—O15^{viii}	103.8 (2)
Na19—O16—K21^{vii}	95.8 (2)	O12—K21—O16^{vii}	71.2 (2)
Na19^{vii}—O16—K21^{vii}	108.3 (2)	O12^{iii}—K21—O14^{vii}	76.41 (19)

C3—O17—H18	103.0 (4)	O12^{iii}—K21—O15^{viii}	155.1 (2)
C3—O17—Na19	108.1 (4)	O12^{iii}—K21—O16^{vii}	100.1 (2)
C3—O17—K20	116.5 (3)	O14^{vii}—K21—O15^{viii}	80.59 (19)
H18—O17—Na19	131.6 (4)	O14^{vii}—K21—O16^{vii}	67.13 (17)
H18—O17—K20	111.0 (3)	O15^{viii}—K21—O16^{vii}	79.24 (16)
Na19—O17—K20	87.0 (2)		

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x-1, y+1, z$; (v) $x, y+1, z$; (vi) $-x+1, -y+2, -z+2$; (vii) $-x+1, -y+2, -z+1$; (viii) $-x, -y+2, -z+1$; (ix) $x+1, y, z$; (x) $x, y-1, z$; (xi) $x+1, y-1, z$.

(ramm090_DFT)

Crystal data

$NaK_2C_6H_5O_7$
$M_r = 290.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.5128$ Å
$b = 7.6258$ Å
$c = 11.3712$ Å
$\alpha = 83.4276°$
$\beta = 88.9910°$
$\gamma = 84.3488°$
$V = 472.59$ Å^3
$Z = 2$
$T = 300$ K

Data collection

Density functional calculation

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.23528	0.68012	0.69007	0.01520*
C2	0.20379	0.79317	0.79461	0.01140*
C3	0.32923	0.96572	0.77770	0.01140*
C4	0.23685	1.08853	0.87187	0.01140*
C5	0.37097	1.25602	0.87268	0.01520*
C6	0.26511	1.06433	0.65294	0.01520*
H7	0.27614	0.71264	0.87452	0.01480*
H8	0.01064	0.82948	0.80961	0.01480*
H9	0.25919	1.01393	0.96018	0.01480*
H10	0.04244	1.12921	0.86015	0.01480*
O11	0.04358	0.63007	0.64853	0.01520*
O12	0.44832	0.64571	0.65042	0.01520*
O13	0.25846	1.38757	0.91438	0.01520*
O14	0.59064	1.25043	0.83476	0.01520*
O15	0.04336	1.07764	0.62268	0.01520*
O16	0.43463	1.12385	0.58916	0.01520*
O17	0.58637	0.92180	0.79054	0.01520*
H18	0.64696	1.03836	0.79618	0.01980*
Na19	0.75225	0.87197	0.59720	0.02020*
K20	0.76524	0.55149	0.86072	0.02970*
K21	0.25613	0.63139	0.41533	0.01970*

Bond lengths (Å)

C1—C2	1.544	C4—C5	1.539
C1—O11	1.274	C4—H9	1.099
C1—O12	1.265	C4—H10	1.092
C2—C3	1.537	C5—O13	1.262
C2—H7	1.095	C5—O14	1.277
C2—H8	1.089	C6—O15	1.267
C3—C4	1.549	C6—O16	1.261
C3—C6	1.557	O17—H18	0.989
C3—O17	1.430		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O17—H18···O14	0.989	1.721	2.614	148.2
C2—H7···O13	1.095	2.480	3.448	165.8
C2—H8···O17	1.089	2.382	3.513	149.0